



**5<sup>th</sup> Symposium of the Los Alamos Computer Science Institute: LACSI 2004 ♦ 12 - 14 October**

**Chair: Dr. Rod Oldehoeft (rro@lanl.gov); Program Chair: Dr. Rob Fowler (rjf@rice.edu)**

**Symposium Site: Eldorado Hotel, 309 West San Francisco Street, Santa Fe, NM 87501**

**\* \* \* \* \***

## **MONDAY, OCT. 11: REGISTRATION/CHECK-IN**

**North Concourse**

**1 PM – 8:00 PM**

**\* \* \* \* \***

## **TUESDAY, OCT. 12: WORKSHOPS & TUTORIALS**

*(Workshops will be held at either the Eldorado or the Hilton. Room assignments appear below.)*

**REGISTRATION/CHECK-IN**

**North Concourse**

**8:00 AM – 8:00 PM**

**CONTINENTAL BREAKFAST**

**Eldorado--North Concourse**

**8:00 – 9:30**

**HILTON HOTEL:**

**(1) Open Source Development and Software Engineering Practices**

**full day**

**Ortiz One**

**9:00 – 12:30**

**(2) Mimetic Methods for PDEs and Applications**

**full day**

**Ortiz Two**

**9:00 – 12:30**

**(3) Python for High Productivity Computing**

**full day**

**Ortiz Three**

**9:00 – 12:30**

**ELDORADO HOTEL:**

**(4) Performance & Productivity of Extreme-Scale Parallel Systems**

**full day**

**Anasazi North**

**9:00 – 12:30**

**(5) Clustermatic: An Innovative Approach to Cluster Computing**

**full day**

**Zia B**

**9:00 – 12:30**

**(6) Path to Extreme Supercomputing**

**full day**

**De Vargas**

**9:00 – 12:30**

**(7) High Availability & Performance Computing**

**full day**

**Zia A**

**9:00 – 12:30**

**(8) Taking Your MPI Application to the Next Level: Threading,  
Dynamic Processes, & Multi-Network Utilization**

**full day**

**Zia C**

**9:00 – 12:30**

**(9) Adaptive Mesh Refinement (AM)**

**half day**

**Sunset Room**

**9:00 – 12:30**

**AM BREAK**

**Eldorado / Hilton**

**10:30: - 11:00**

**LUNCH**

**(on your own)**

**12:30 – 2:00**



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REGISTRATION/CHECK-IN	North Concourse		8:00 AM – 8:00 PM
HILTON HOTEL:			
(1) Open Source Development and Software Engineering Practices	concluded	Ortiz One	2:00 – 5:30
(2) Mimetic Methods for PDEs and Applications	concluded	Ortiz Two	2:00 – 5:30
(3) Python for High Productivity Computing	concluded	Ortiz Three	2:00 – 5:30
ELDORADO HOTEL:			
(4) Performance & Productivity of Extreme-Scale Parallel Systems	concluded	Anasazi North	2:00 – 5:30
(5) Clustermatic: An Innovative Approach to Cluster Computing	concluded	Zia B	2:00 – 5:30
(6) Path to Extreme Supercomputing	concluded	De Vargas	2:00 – 5:30
(7) High Availability & Performance Computing	concluded	Zia A	2:00 – 5:30
(8) Taking Your MPI Application to the Next Level: Threading, Dynamic Processes, & Multi-Network Utilization	concluded	Zia C	2:00 – 5:30
(10) Building Scalable Simulations of Complex Socio-Technical Systems (PM)	half day	Sunset Room	2:00 – 5:30
PM BREAK	Eldorado / Hilton		3:30 – 4:00
POSTERS SET-UP (push pins & boards provided, 1 panel each)	Anasazi Ballroom South		3:00 – 5:00
WELCOME RECEPTION/POSTER EXHIBIT	Anasazi Ballroom South		6:00 – 7:00



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## **WORKSHOPS & TUTORIALS (12 OCT., TUESDAY)**

**NOTE: #1-8 are full-day workshops; #9 & 10 are half-day workshops.**

**All workshops will be held at the Eldorado OR the Hilton (across the street).**

**Room assignments are posted**

### **(1) OPEN SOURCE DEVELOPMENT AND SOFTWARE ENGINEERING Practices**

**(full day)**

***Rod Oldehoeft (rro@lanl.gov; 505-665-3663)***

Many organizations have established standard practices in software engineering (SE) for their projects. These are often predicated on a traditional view of an in-house team of employees with a common project goal. However, in other organizations, reliance on, and contributing to, open-source software (OSS) is important. In this world, software development processes have some different origins, goals, and outputs than traditional SE processes. This workshop will explore the implications of these different but co-existing worldviews. Speakers include DOE lab project managers and software developers, and well-known researchers studying open-source development phenomena. The result will be a better understanding of issues, not a "silver bullet."

### **(2) MIMETIC METHODS FOR PDES AND APPLICATIONS**

**(full day)**

***Mikhail Shashkov (Shashkov@lanl.gov; 505-667-4400)***

Mimetic methods are the class of methods that mimic important properties of underlying geometrical, mathematical and physical models, such as geometry, conservation laws, symmetry preservation, positivity and monotonicity preservation. This workshop is focused on presentation of new mimetic discretizations for wide variety of partial differential equations (PDE).



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### **(3) PYTHON FOR HIGH PRODUCTIVITY COMPUTING**

**(full day)**

***Craig E. Rasmussen (rasmussn@lanl.gov; 505-665-6021)***

**A growing trend in the scientific community is to prototype research concepts using Python. This is motivated by very practical reasons: it is free, available on nearly all platforms, provides easy interoperability with other languages, and has a mature base of scientific extension libraries. This workshop will bring together users and developers to explore the use of Python in scientific computing. The workshop will focus on programmer productivity, with a tutorial session in the AM & a technical session in the PM.**

### **(4) PERFORMANCE AND PRODUCTIVITY OF EXTREME-SCALE PARALLEL SYSTEMS**

**(full day)**

***Adolfy Hoisie (hoisie@lanl.gov; 505-667-5216)***

**Building extreme-scale parallel systems and applications that can achieve high performance has proven to be incredibly difficult. Today's systems have complex processors, deep memory hierarchies and heterogeneous interconnects requiring careful scheduling of an application's operations, data accesses and communication to achieve a significant fraction of potential performance. Furthermore, the large number of components in extreme-scale parallel systems makes component failure inevitable; therefore, achieving fault-tolerance in hardware and/or system software becomes an integral part of the performance landscape. In addition to "classical" performance considerations, the notion of high productivity of systems at scale is now of paramount importance. Productivity encompasses availability, fault tolerance, ease of use, upward portability (including performance portability), as well as code development time. The latter is not a focus of our workshop.**



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## **WORKSHOPS & TUTORIALS (12 OCT., TUESDAY)**

### **(5) CLUSTERMATIC: AN INNOVATIVE APPROACH TO CLUSTER COMPUTING**

**(full day)**

***Gregory Watson (gwatson@lanl.gov; 505-665-0726)***

Clustermatic is an award winning, innovative, software architecture that redefines cluster computing at all levels--from the BIOS to the parallel environment. Other cluster systems typically rely on a complicated software suite that is layered on top of a conventional operating system that must be installed on a local disk in every node. The complexity and size of these systems tends to limit their deployment to small-to-mid size machines, reduces reliability, and requires a significant management overhead for normal administrative activities. In contrast, the Clustermatic design maximizes performance and availability by achieving significant improvements in system booting and application startup times, minimizing points of failure and vastly simplifying management and administration activities. It is suitable for use on a wide range of architectures, and has been successfully deployed on tiny clusters containing only 2 diskless nodes all the way up to a 1408 node (2816 processor), 11 Tflop cluster at Los Alamos National Laboratory. Key components of Clustermatic include LinuxBIOS, BProc, BJS, LA-MPI, and Linux.

### **(6) PATH TO EXTREME SUPERCOMPUTING**

**(full day)**

***Erik P. DeBenedictis (epdeben@sandia.gov; 505-284-4017)***

Applications scientists envision applications for supercomputers up to 1 Zettaflops ( $10^{21}$  FLOPS), yet there is little consensus on how to build them. Recent studies of computational science applications show a continuum of truly important problems requiring supercomputers from today's 40 Teraflops to 1 Zettaflops over a period of several decades. This represents a faster growth than the historical trend of supercomputer performance. Furthermore, this magnitude of supercomputer performance exceeds the limits set by the laws of physics for clusters and Massively Parallel Processors (MPP). In this workshop, scientists will describe the limits of current computers and propose a constructive path for extending supercomputer power to meet applications demand. The purpose of the workshop is to inform participants of the issues and provide a basis for interdisciplinary cooperation.



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## **WORKSHOPS & TUTORIALS (12 OCT., TUESDAY)**

### **(7) HIGH AVAILABILITY AND PERFORMANCE COMPUTING**

**(full day)**

***Stephen L. Scott (scottsl@ornl.gov; 865-574-3144)***

HAPCW2004 is a forum for state-of-art and on-going research in High-Availability and Performance Computing. High-Availability (HA) Computing has long played a critical role in commercial mission critical applications. Likewise, High-Performance Computing (HPC) has equally been a significant enabler of the R&D community for scientific discoveries. Serviceability aims toward effective means by which corrective and preventive maintenance can be performed on a system. Higher serviceability improves availability and helps sustaining quality, performance and continuity of services at expected levels. Together, the combination of HA, Serviceability, and HPC will clearly lead to even more benefits to critical shared major HEC resource environments. Papers will be electronic-published on the web site and CD.

### **(8) TAKING YOUR MPI APPLICATION TO THE NEXT LEVEL: THREADING, DYNAMIC PROCESSES, & MULTI-NETWORK UTILIZATION**

**(full day)**

***Richard L. Graham (rlgraham@lanl.gov; 505-665-5685)***

Important features of the MPI-2 specification and run-time environments have only recently matured in MPI implementations. Multi-threaded MPI programs can be exploited for useful control and computational features. MPI-2 dynamic process models can be used for practical applications such as dynamically reporting on the status of long-running parallel codes. Using multiple networks to communicate between processes is becoming increasingly relevant in both the LAN and Grid/WAN environments. Finally, run-time tuning of the MPI implementation itself allows performance tweaking without changing any application code. A balance of presentation and hands-on examples aimed at users, system administrators, and developers will be used.



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## **WORKSHOPS & TUTORIALS (12 OCT., TUESDAY)**

### **(9) ADAPTIVE MESH REFINEMENT**

**(half day AM)**

***Bobby Philip (bphilip@lanl.gov; 505-667-3844); Michael Pernice (pernice@lanl.gov; 505-665-7119)***

The demand for greater accuracy, detail, and complexity in computational science cannot be satisfied solely by hardware advances. In numerical simulations, AMR can provide increased local resolution at greatly reduced cost. Using AMR has historically been time-consuming and application-specific, limiting its use. The workshop will highlight challenges in making AMR technology more accessible to the scientific community. Issues of interest include optimal parallel solver capabilities, interfacing frameworks with application codes, and interoperability of different frameworks. The workshop will provide a forum for AMR framework and application developers to highlight and propose solutions to some of these problems.

### **(10) BUILDING SCALABLE SIMULATIONS OF COMPLEX SOCIO-TECHNICAL SYSTEMS**

**(half day, PM)**

***James P. Smith (jpsmith@lanl.gov; 505-665-0921)***

Complex socio-technical systems consist of a large number of interacting physical, technological, and human/societal components. Examples of such systems are urban regional transportation systems, national electrical powermarkets and grids, the Internet, ad-hoc communication and computing systems, public health, etc. Realistic social and infrastructure networks spanning urban regions are extremely large: consisting of millions of nodes and edges. As a result, the detailed simulations capable of representing such systems consist of millions of interacting agents. The challenges pertaining to design and implementations of such simulations on high performance computing platforms are unique, e.g., computation of extremely large dynamic unstructured composed networks. The workshop aims to bring together some of the leading researchers with the goal of identifying fundamental issues in designing, implementing and using such simulations on current and next generation high performance computing architectures. Examples of topics that will be covered include scalable HPC oriented design of such simulations; distributed algorithms and their implementations; formal specifications and simulation specific HPC system software.

**WELCOME RECEPTION/POSTER EXHIBIT**

**Anasazi Ballroom South**

**6:00 – 7:00**



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## **POSTER EXHIBITS (12 – 14 Oct., Tues-Thurs)**

***Posters will be set up in the Anasazi Ballroom South during the PM Break, 12 Oct., Tues. (3:30-4:00) and at the end of the day (5:00-6:00). The Welcome Reception/Poster Exhibit will be held from 6:00 to 7:00.***

### ***Using Generic Programming Techniques with Procedural Finite Element Codes***

**Fehmi Cirak and Julian C. Cummings (California Institute of Technology)**

### ***Cost-effective Performance-scalable Workstation Accelerators for High-resolution Volumetric Imaging***

**Robert Michael Lea, Aby Jacob Abraham, and Pawel Tomil Tetnowski (School of Engineering & Design, Brunel University, UK)**

### ***Reliability, Availability and Serviceability Management for HPC Linux Clusters: Self-awareness Approach***

**Stephen L Scott (ORNL); Chokchai Leangsuksun, Tong Liu, and Yudan Liu (Louisiana Tech University); Richard Libby (Intel); Ibrahim Haddad (Ericsson Research)**

### ***Design and Development of High Performances Parallel Particle in Cell (PIC)***

**Stefano Markidis, Giovanni Lapenta, and W. Brian VanderHeyden (LANL)**

### ***MPI Collective Operation Performance Analysis***

**Jelena Pjesivac-Grbovic, Thara Angskun, George Bosilca, Graham Fagg, Edgar Gabriel, and Jack Dongarra (Innovative Computing Laboratory, University of Tennessee, Knoxville)**

### ***High Performance Simulation of Developmental Biology on a Hybrid Grid***

**Frederic R. Fairfield (Fairfield Enterprises); Giovanni Lapenta and Stefano Markidis (LANL)**

### ***A Sample-Driven Call Stack Profiler***

**Nathan Froyd, John Mellor-Crummey, and Robert J. Fowler (Rice University)**

### ***Reliability Costs in LA-MPI***

**Galen M. Shipman, Arthur B. Maccabe, and Patrick G. Bridges (The University of New Mexico)**

### ***Design and Implementation of Adifor90: Preliminary Results***

**Michael Wayne Fagan (Rice University)**



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## **WEDNESDAY, OCT. 13: KEYNOTE ADDRESS & RESEARCH PAPERS**

**(Sessions convene in Anasazi Ballroom; registration/check-in continue in North Concourse.)**

**CONTINENTAL BREAKFAST** **North Concourse** **8:00 – 9:30**

**Welcome: Andy White, LANL, & Ken Kennedy, Rice University,** **9:00 – 9:30**  
**LACSI Co-Directors**

**Keynote: *On Demand Processing, Query, and Exploration of Distributed Petascale Datasets***

**Dr. Joel Saltz, MD, PhD, Chair and Professor Biomedical Informatics** **9:30–10:30**  
**Professor Computer Science, Pathology, The Ohio State University**

**AM BREAK** **North Concourse** **10:30 – 11:00**

**Research Papers: Systems** **11:00 - 12:30**

***How To Build A Fast And Reliable 1024 Node Cluster With Only One Disk***

**Erik Arjan Hendriks and Ronald Minnich (LANL)**

***An Event-driven Architecture for MPI Libraries***

**Supratik Majumder and Scott Rixner (Rice University); Vijay S. Pai (Purdue University)**

***Layout Transformation Support for the Disk Resident Arrays Framework***

**Sriram Krishnamoorthy, Gerald Baumgartner, Chi-Chung Lam, and P. Sadayappan (The Ohio State University); Jarek Nieplocha (Pacific Northwest National Laboratory)**

**LUNCH** **(on your own)** **12:30 – 2:00**



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## **WEDNESDAY, OCT. 13: KEYNOTE ADDRESS & RESEARCH PAPERS (concluded)**

**(Sessions convene in Anasazi Ballroom; registration/check-in continue in North Concourse.)**

### **Research Papers: Compilation and Program Transformation 2:00 – 3:30**

*Exploring the Structure of the Space of Compilation Sequences Using Randomized Search Algorithms*

Keith D. Cooper, Alexander Grosul, Timothy J. Harvey, Steve Reeves, Devika Subramanian,  
Linda Torczon, and Todd Waterman (Rice University)

*Experiences with Sweep3D Implementations in Co-array Fortran*

Cristian Coarfa, Yuri Dotsenko, and John Mellor-Crummey (Rice University)

*Automatic Tuning of Whole Applications Using Direct Search and a Performance-based Transformation System*

Apan Qasem, Ken Kennedy, and John Mellor-Crummey (Rice University)

### **PM BREAK North Concourse 3:30 – 4:00**

### **Research Papers: Applications and Performance 4:00 – 5:30**

*Rapid Prototyping Frameworks for Developing Scientific Applications: A Case Study*

Christopher D. Rickett (South Dakota School of Mines and Technology); Sung-Eun Choi,  
Craig E. Rasmussen, and Matthew J. Sottile (LANL)

*On the Use of a Two-Grids Method in the Numerical Simulation of Free Boundary Problems*

Alexandre Caboussat and Roland Glowinski (University of Houston)

*Memory Performance Profiling via Sampled Performance Monitor Event Traces*

Diana Villa, Jaime Acosta, and Patricia Teller (The University of Texas at El Paso);  
Bret Olszewski (IBM Corp.); Trevor Morgan (Exxon/Mobil Corp.)

### **ADJOURNMENT 5:30**



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## **THURSDAY, OCT. 14: PANEL DISCUSSIONS**

**(Panels convene in Anasazi Ballroom; registration/check-in continue in North Concourse.)**

### **CONTINENTAL BREAKFAST**

**North Concourse**

**8:00 – 9:30**

#### **Panel I: FPGAs in High Performance Computing**

**9:00 – 10:30**

**Use of Field-Programmable Gate Arrays is expanding from specialized embedded systems to more general-purpose application accelerators. Panelists will consider software support aspects and applications using FPGAs. Moderator: Rod Oldehoeft, LANL**

**Wim Bohm, Colorado State University**

**Maya Gokhale, Los Alamos National Laboratory**

**Jeffrey Hammes, SRC Computers, Inc.**

**Burton Smith, Cray, Inc.**

**Scott Hemmert, Sandia National Laboratories**

### **AM BREAK**

**North Concourse**

**10:30: - 11:00**

#### **Panel II: Computer Science Innovations in ASC ASAP Centers**

**11:00 – 12:30**

**The ASC Academic Strategic Alliance Program Centers pursue advances in computational science, computer systems, mathematical modeling, and numerical mathematics important to Advanced Simulation and Computing. The panelists will discuss innovations in computer science that are contributing to the success of their Centers. Moderator: Karl-Heinz A. Winkler, LANL**

**Michael Aivazis, California Institute of Technology**

**Eric Darve, Stanford University**

**Anshu Dubey, University of Chicago**

**Tom Henderson, University of Utah**

**Laxmikant Kale, University of Illinois  
at Urbana-Champaign**

### **LUNCH (on your own)**

**12:30 – 2:00**



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**THURSDAY, OCT. 14: PANEL DISCUSSIONS (concluded)**

**(Panels convene in Anasazi Ballroom; registration/check-in continue in North Concourse.)**

**Panel III: HPC Languages of the Future** **2:00 – 3:30**

**Moderator: Robert J. Fowler, Rice University**

**David Chase, Sun**

**John Mellor-Crummey, Rice University**

**Vivek Sarkar, IBM**

**Burton Smith, Cray, Inc.**

**PM BREAK** **North Concourse** **3:30 – 4:00**

**Panel IV: Whither High Performance Computing? (Open panel)** **4:00 - 5:30**

**An opportunity for participants to offer their views & opinions regarding future directions in HPC.**

**We encourage presentations on the following –**

- **Industry perspectives, technological and economic**
- **Government support issues**
- **Emerging problems, crises, and catastrophes**
- **Advocacy for specific initiatives, both technical and programmatic**

**Format: 5 min. per speaker**

- **After each group of 3 presentations, there will be 10 min. of questions & followup.**

**A signup sheet will be available through the end of symposium activities on Wed., Oct 13.**

**CLOSING RECEPTION** **Sunset Room** **5:30 – 7:00**

***THANK YOU FOR ATTENDING LACSI 2004.***

***SEE YOU AT LACSI 2005!***